LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
Acq On : 1 Sep 2018 7:22
Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.672	560	567	568	rBV2	28548	52435	2.22%	0.395%
2	6.660	728	735	739	rBV	49139	98169	4.16%	0.739%
3	6.772	751	754	789	rVV	361278	965990	40.94%	7.269%
4	7.007	790	794	815	rVV	124473	384572	16.30%	2.894%
5	7.154	815	819	872	rVB	1110342	1889928	80.10%	14.222%
6	7.566	885	889	912	rBV	399364	1142849	48.44%	8.600%
7	8.284	1007	1011	1040	rBV	141403	406856	17.24%	3.062%
8	9.348	1189	1192	1220	rBV	1392091	2224254	94.27%	16.737%
9	9.742	1253	1259	1264	rBV	39985	61867	2.62%	0.466%
10	10.042	1306	1310	1322	rBV	270096	395534	16.76%	2.976%
11	10.695	1418	1421	1428	rVB	33475	40203	1.70%	0.303%
12	10.836	1441	1445	1457	rBV	354683	719934	30.51%	5.417%
13	11.542	1561	1565	1587	rBV	251109	477093	20.22%	3.590%
14	13.119	1829	1833	1855	rBV	1975453	2359342	100.00%	17.754%
15	13.319	1864	1867	1872	rBV	46533	41551	1.76%	0.313%
16	13.660	1922	1925	1928	rBV	76124	72339	3.07%	0.544%
17	13.989	1978	1981	1989	rVB	102245	94972	4.03%	0.715%
18	14.195	2012	2016	2026	rBV	371826	537475	22.78%	4.044%
19	14.307	2031	2035	2039	rBV	148834	124057	5.26%	0.934%
20	14.613	2084	2087	2091	rBV	157777	134457	5.70%	1.012%
21	14.936	2138	2142	2149	rBV	134450	147238	6.24%	1.108%
22	15.018	2152	2156	2161	rVB	50026	53520	2.27%	0.403%
23	15.295	2199	2203	2212	rBV	112860	150310	6.37%	1.131%
24	15.707	2268	2273	2276	rBV	100585	137632	5.83%	1.036%
25	15.754	2276	2281	2291	rVB	181577	331644	14.06%	2.496%
26	16.171	2347	2352	2358	rBV	73520	118282	5.01%	0.890%
27	16.718	2440	2445	2451	rBV	46587	81128	3.44%	0.610%
28	17.365	2550	2555	2565	rVB3	19866	45594	1.93%	0.343%

Sum of corrected areas: 13289225

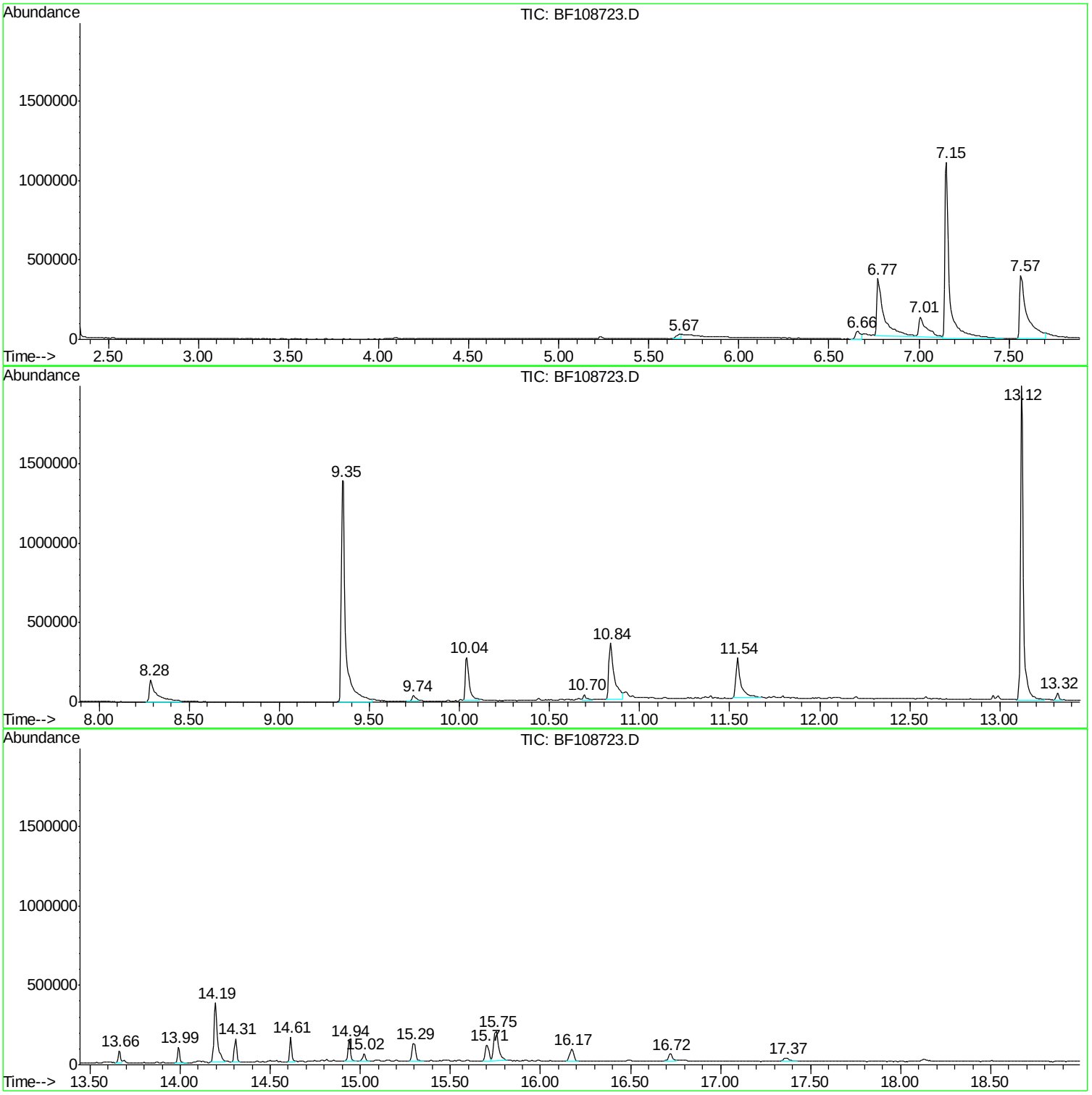
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
Acq On : 1 Sep 2018 7:22
Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
Acq On : 1 Sep 2018 7:22
Operator : JU/SJ
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Misc :
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ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

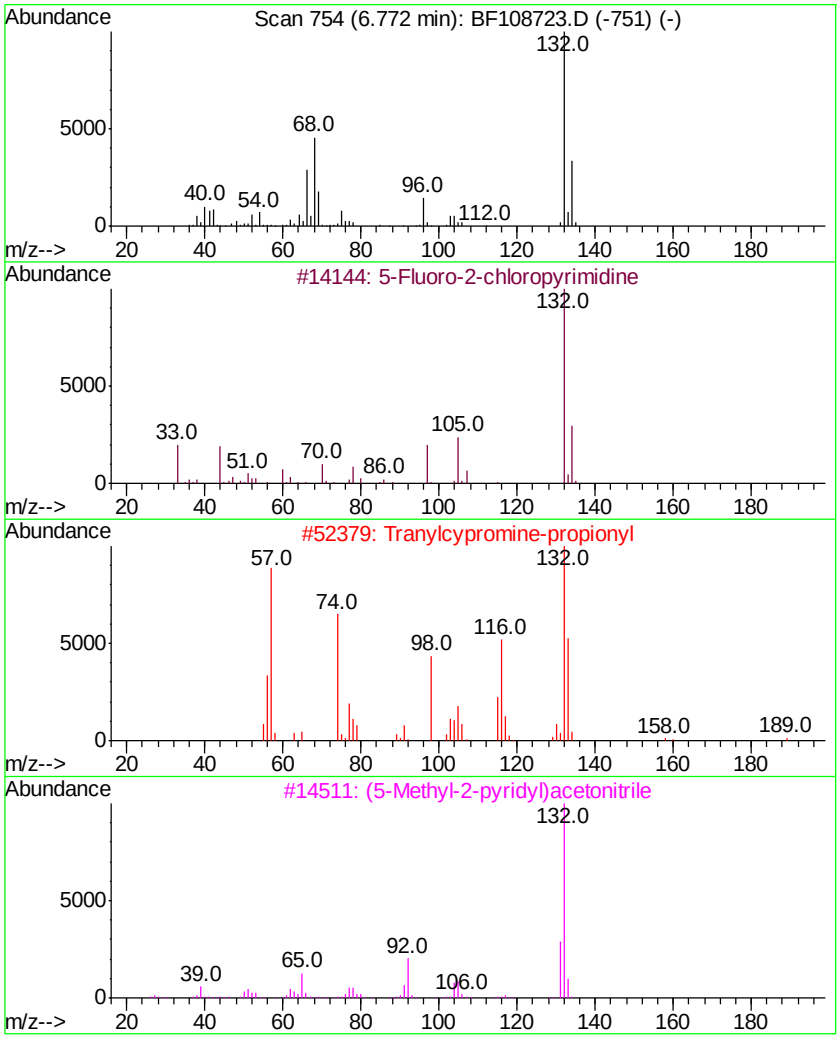
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

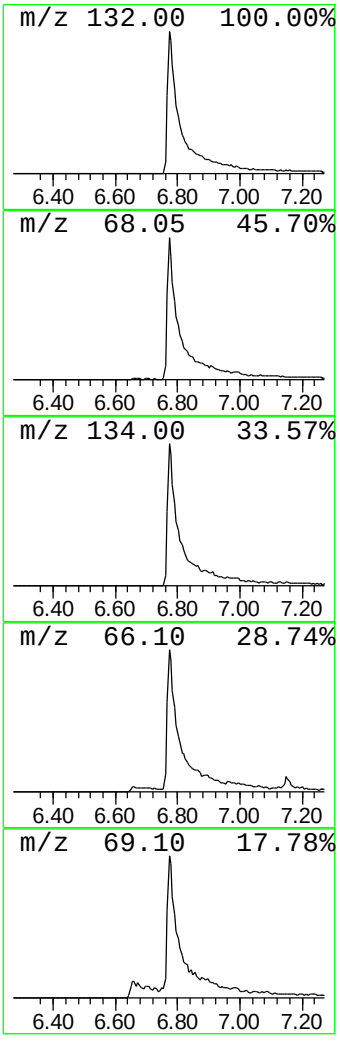
****

Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	50.24 ng	965990	1,4-Dichlorobenzene-d4	7.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
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Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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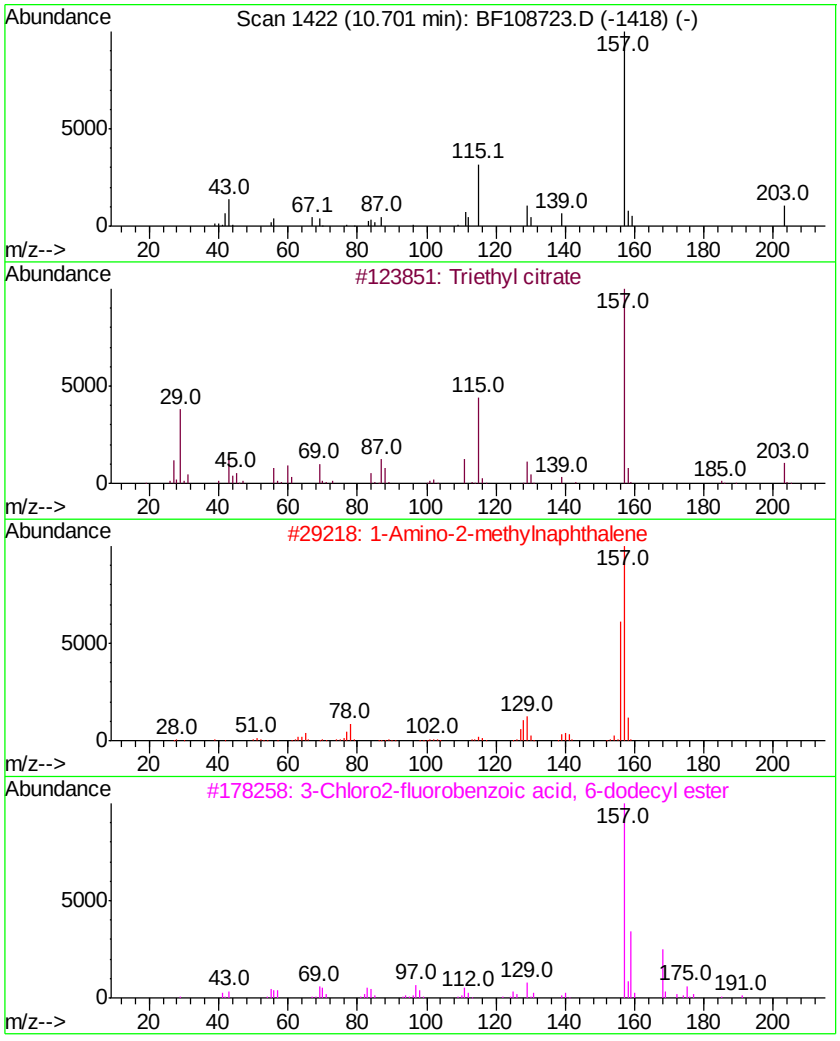
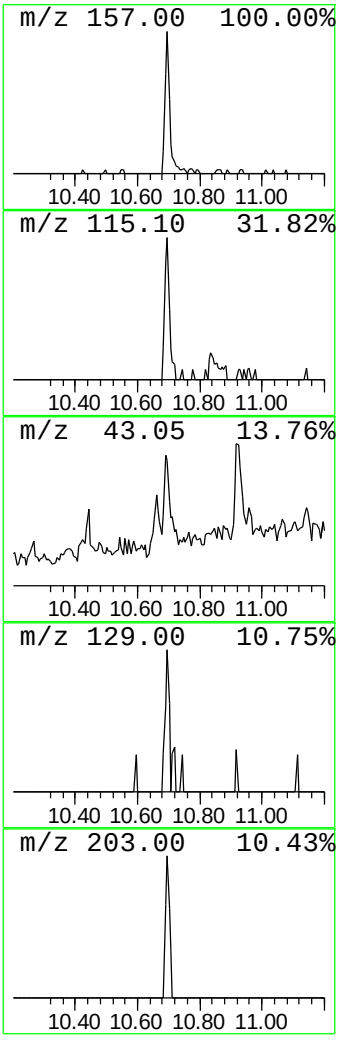
Peak Number 3 Triethyl citrate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.03 ng	40203	Acenaphthene-d10	10.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	83
2	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	50
3	3-Chloro2-fluorobenzoic acid, 6-...	342	C19H28ClFO2	1000338-64-1	38
4	3-Chloro2-fluorobenzoic acid, 4-...	356	C20H30ClFO2	1000338-64-4	36
5	3-Chloro2-fluorobenzoic acid, 3-...	342	C19H28ClFO2	1000338-63-8	36





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Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

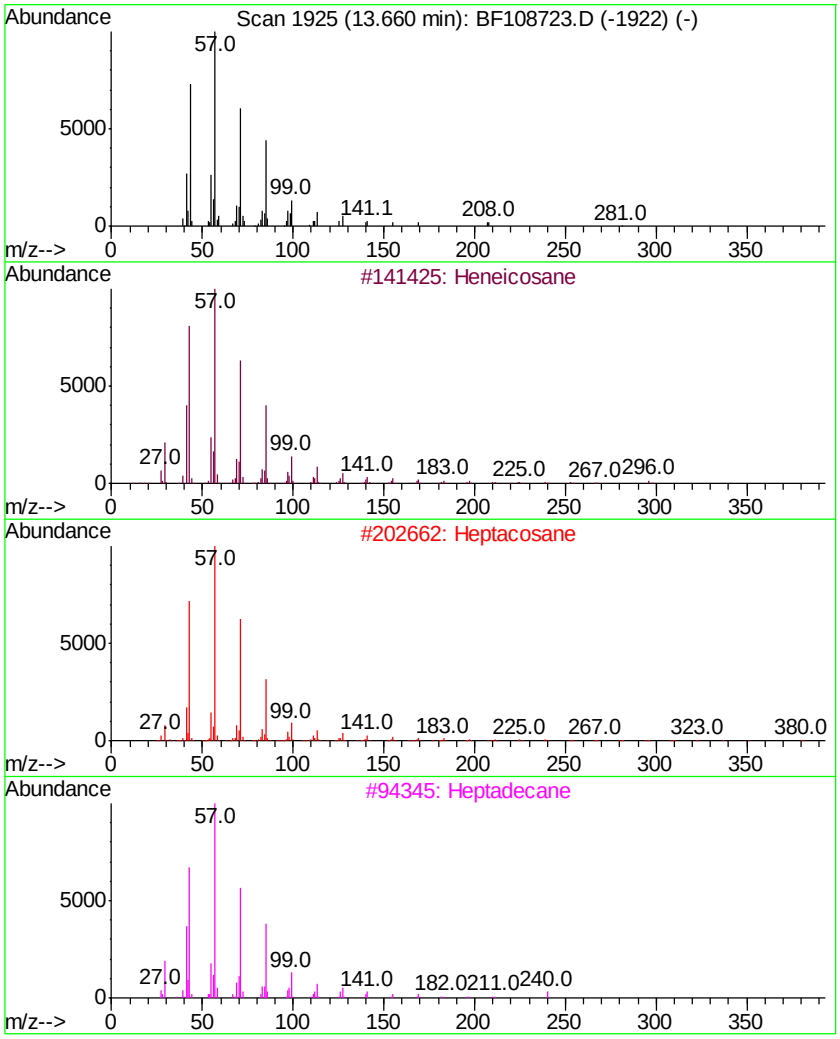
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

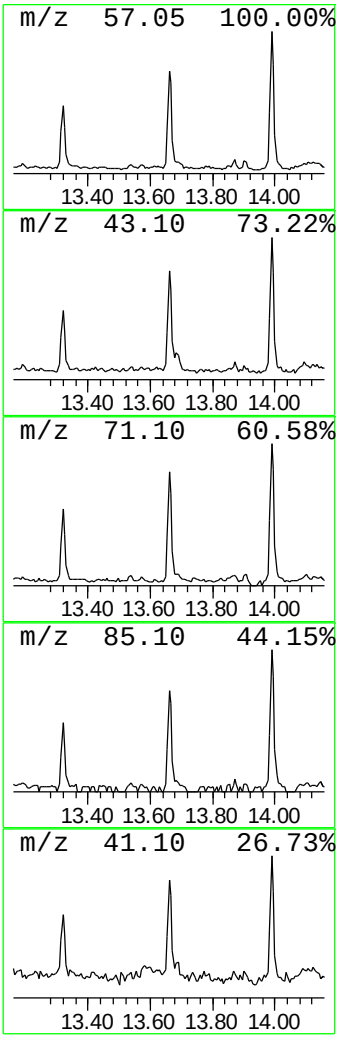
****

Peak Number 4 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	2.69 ng	72339	Chrysene-d12	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Hexadecane	226	C16H34	000544-76-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
Acq On : 1 Sep 2018 7:22
Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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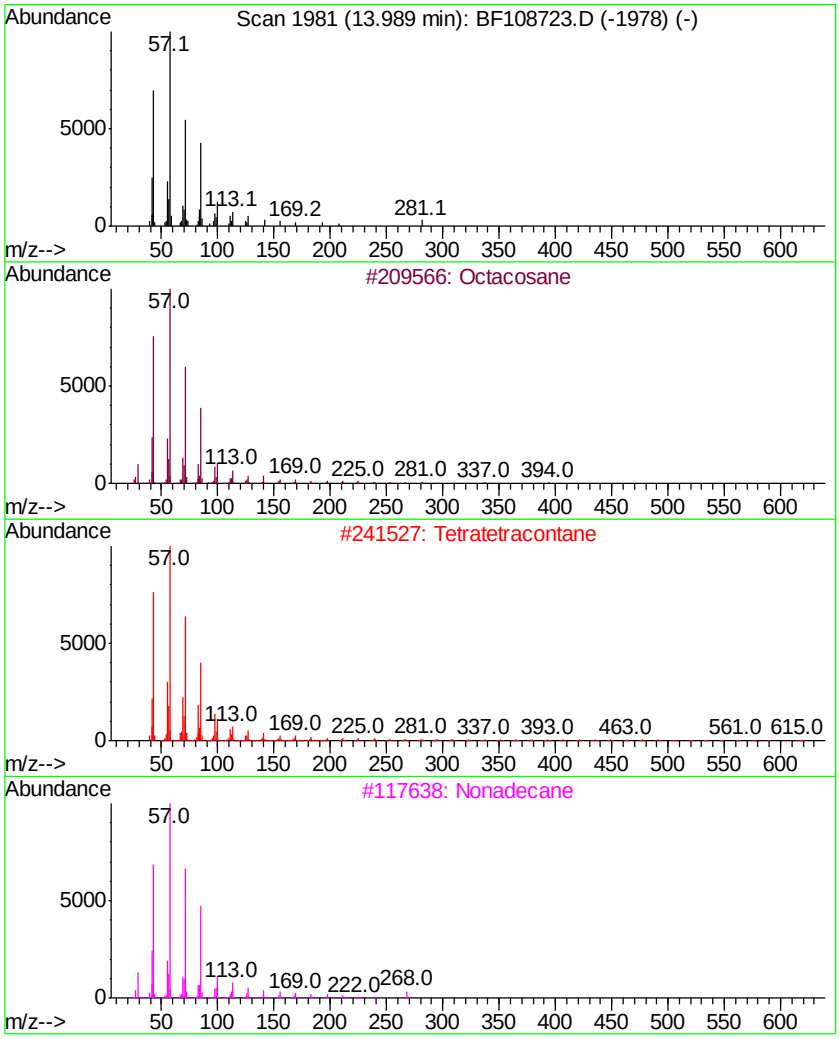
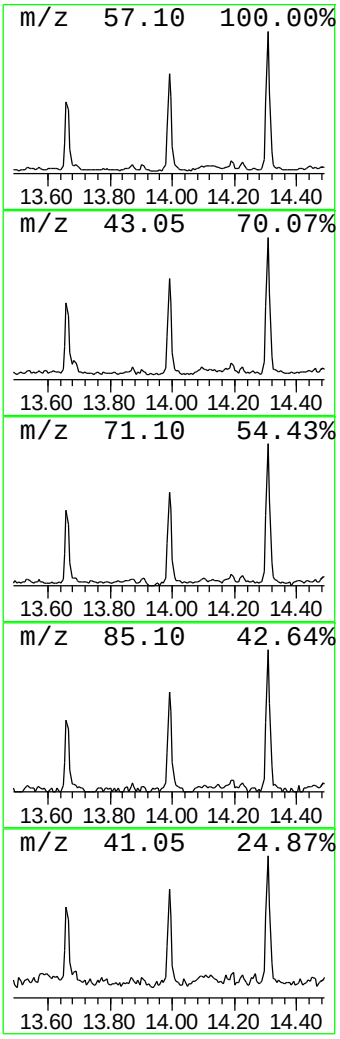
Peak Number 5 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	3.53 ng	94972	Chrysene-d12	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Tetradecane	198	C14H30	000629-59-4	87
5	Pentadecane	212	C15H32	000629-62-9	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108723.D
Acq On : 1 Sep 2018 7:22
Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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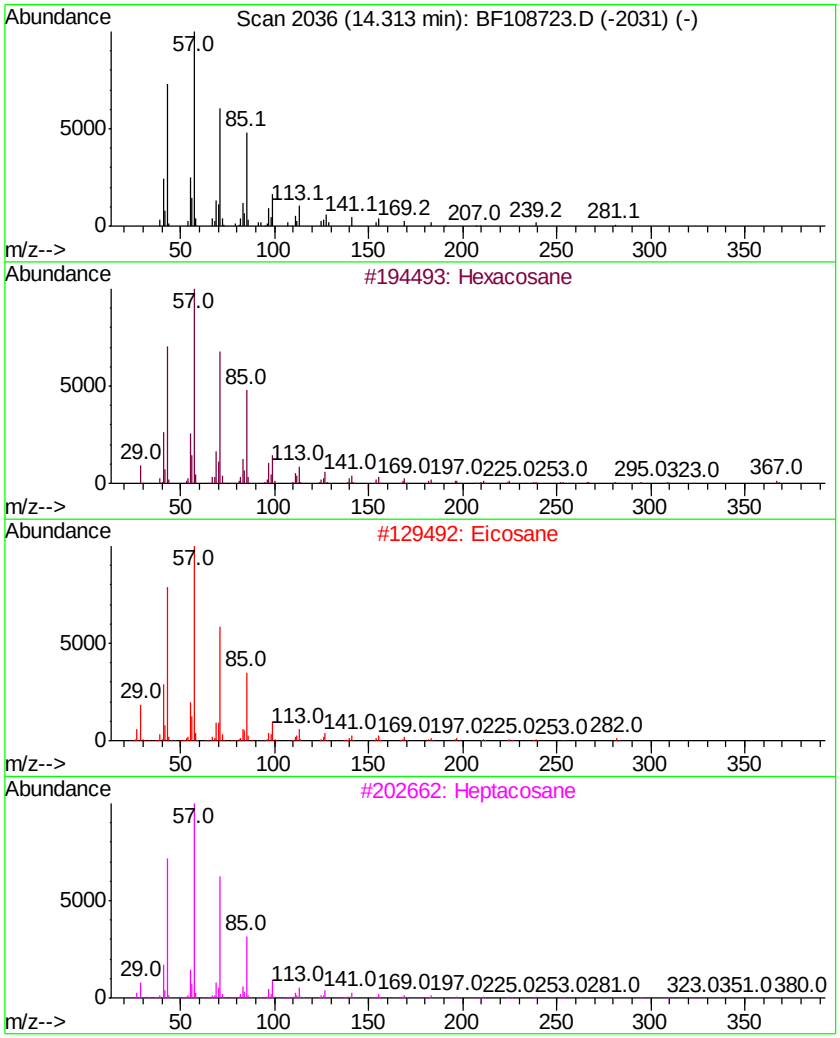
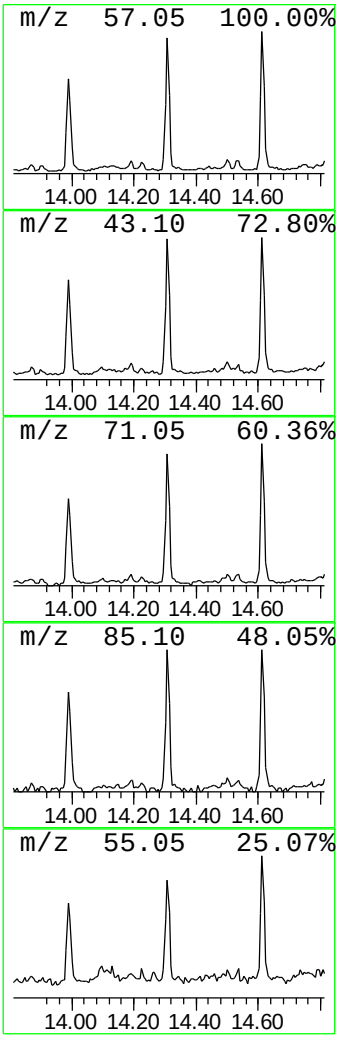
Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	4.62 ng	124057	Chrysene-d12	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	91





Library Search Compound Report

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Operator : JU/SJ
Sample : J4729-09
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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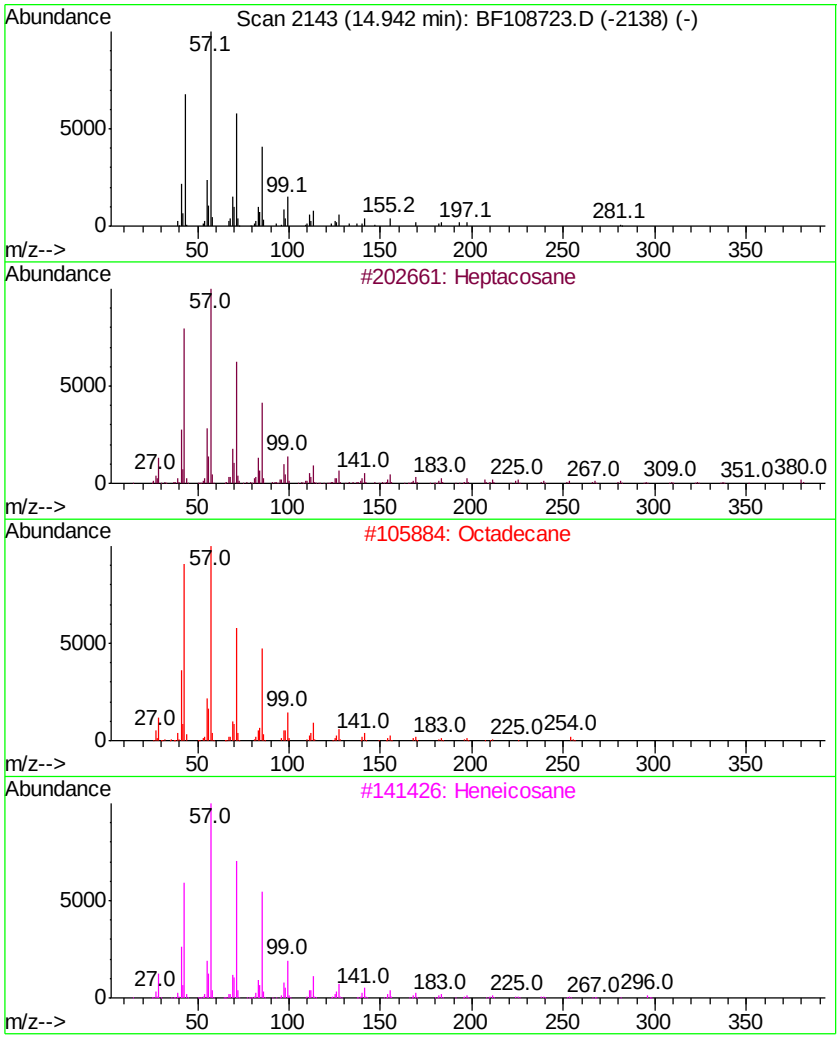
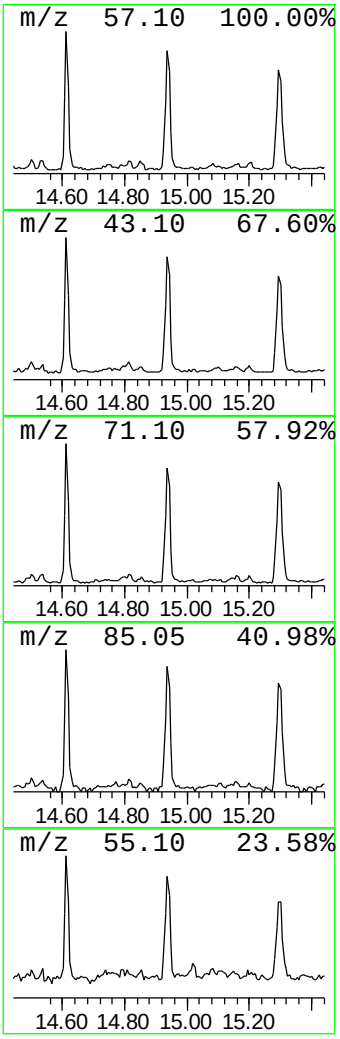
Peak Number 8 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	5.48 ng	147238	Chrysene-d12	14.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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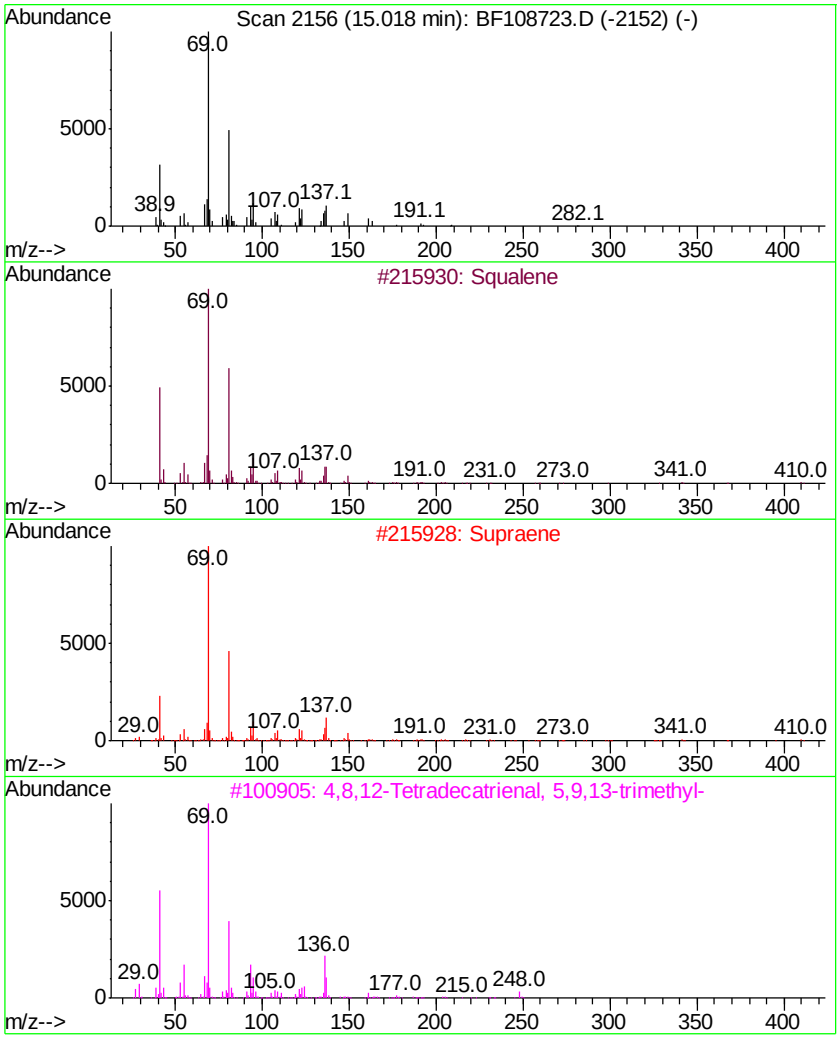
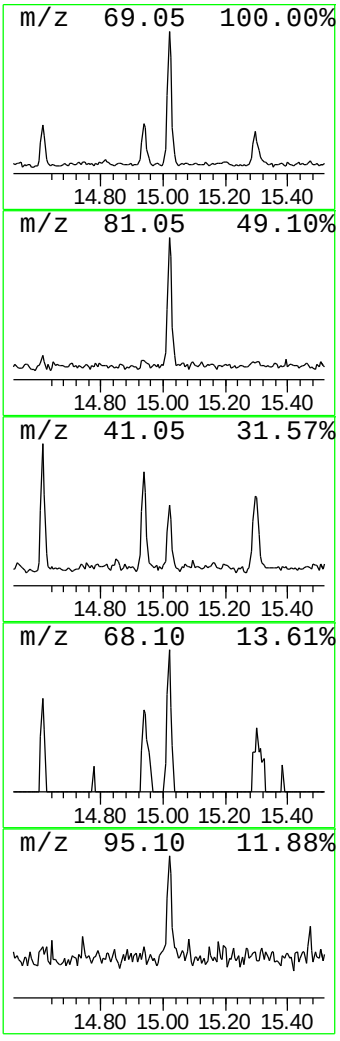
Peak Number 9 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.23 ng	53520	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59





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TIC Library : C:\DATABASE\NIST11.L
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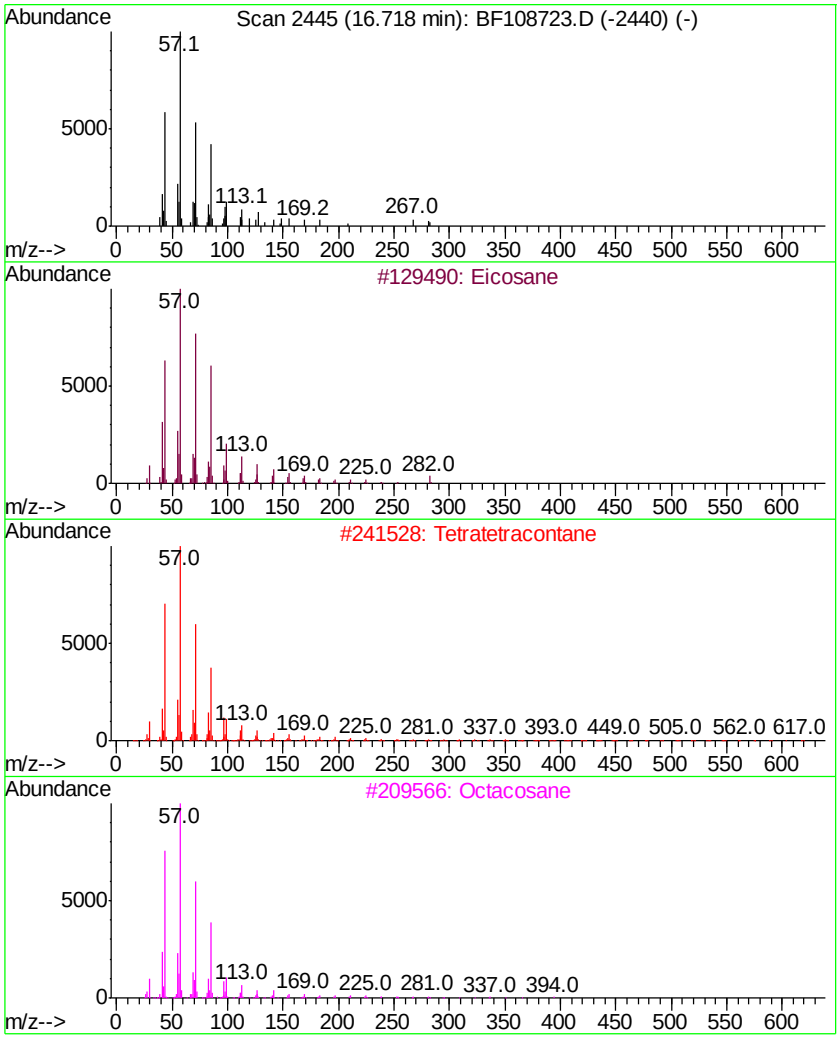
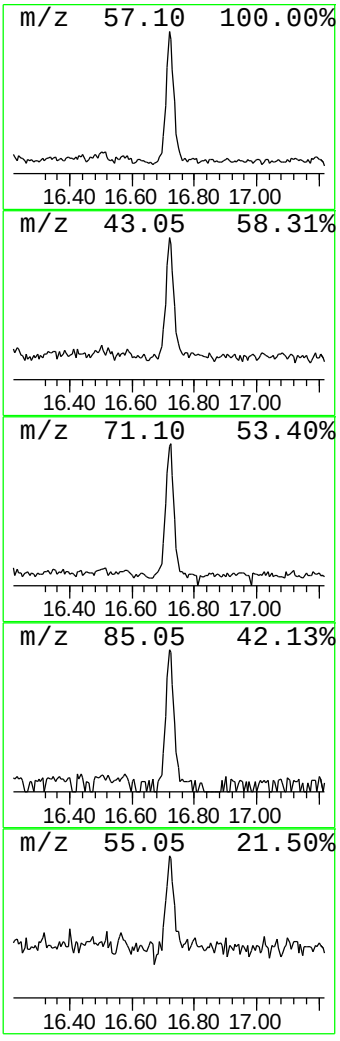
Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	4.89 ng	81128	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





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Sample : J4729-09
Misc :
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Instrument : BNA_F
ClientSampleId : 082918-DBRI-F-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

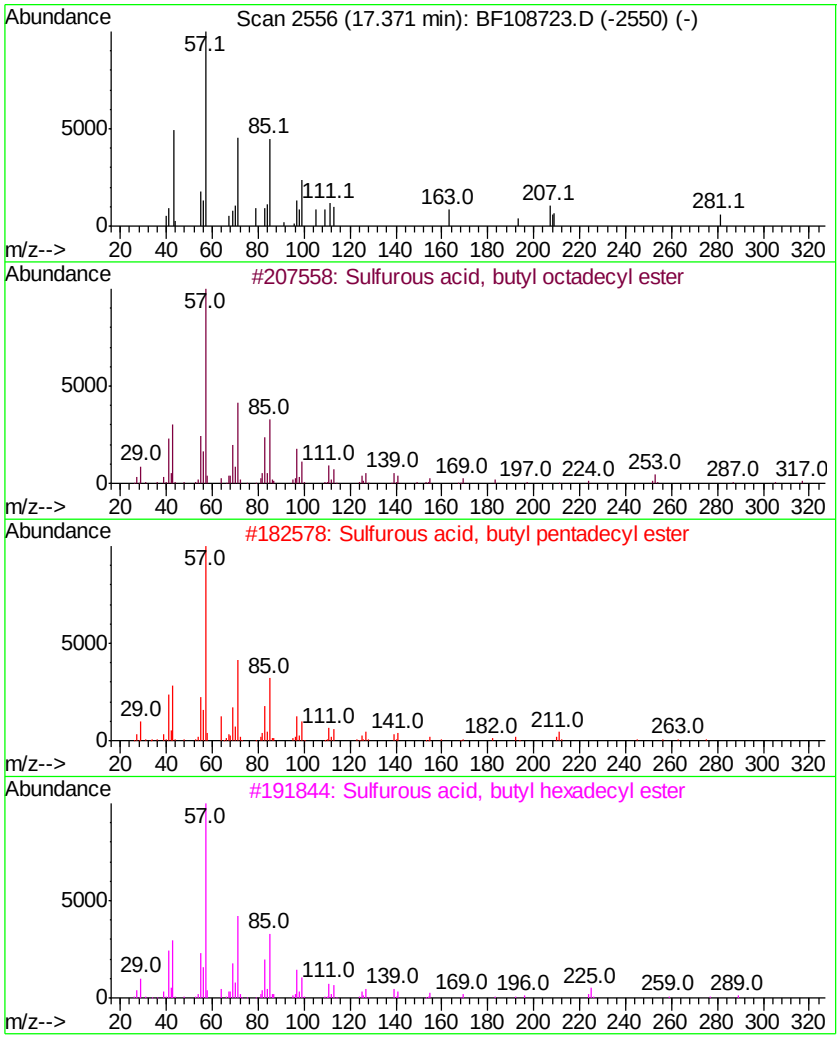
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

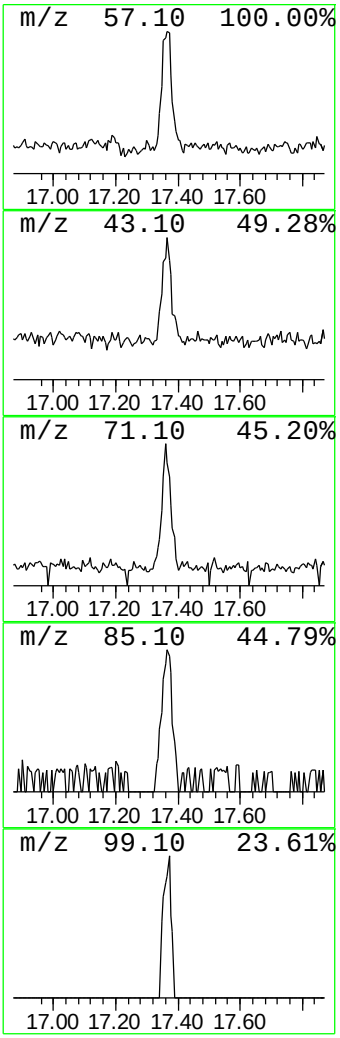
****

Peak Number 13 Sulfurous acid, butyl octad... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	2.75 ng	45594	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	59
2	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	59
3	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	59
4	Hexatriacontane	507	C36H74	000630-06-8	53
5	Tetracosane	338	C24H50	000646-31-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.77	6.77	50.2	ng	965990	1	7.01	384572	20.0
Triethyl citrate	10.70	2.0	ng	40203	3	10.04	395534	20.0
Heneicosane	13.66	2.7	ng	72339	5	14.20	537475	20.0
Octacosane	13.99	3.5	ng	94972	5	14.20	537475	20.0
Hexacosane	14.31	4.6	ng	124057	5	14.20	537475	20.0
Heptacosane	14.94	5.5	ng	147238	5	14.20	537475	20.0
Squalene	15.02	3.2	ng	53520	6	15.75	331644	20.0
Eicosane	16.72	4.9	ng	81128	6	15.75	331644	20.0
Sulfurous acid, b...	17.37	2.8	ng	45594	6	15.75	331644	20.0